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Data Provenance Hybridization Supporting Extreme-Scale Scientific Workflow Applications

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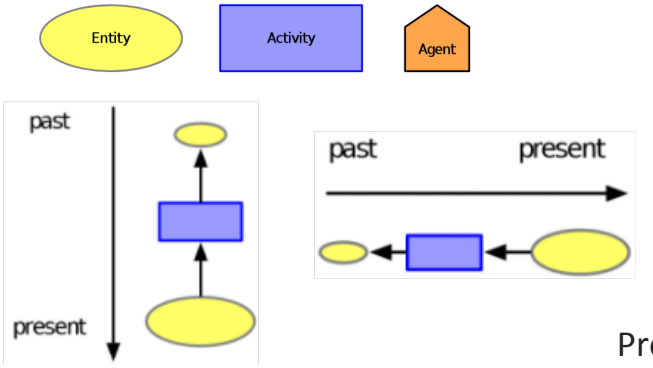
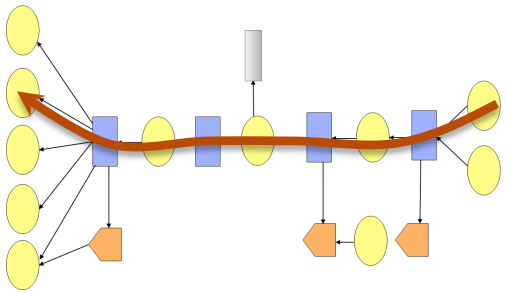
2016 Earth System Grid Federation (ESGF) Workshop

U.S. DEPARTMENT OF ENERGY

Provenance Definitions

- A computable and semantically meaningful historical explanation of influential factors, process flows, and data flows.
- Provenance is information about entities, activities, and people involved in producing a piece of data or thing, which can be used to form assessments about its quality, reliability or trustworthiness [W3C PROV].
- *Disclosure – evidence provided from the perspective of the running application.*
- *Observation* – measurements collected about the computational environment while disclosure is taking place.





Provenance Graph
Tracing Data Origin

Provenance at scale

- **Minimize impact,** control granularity (coarse to fine) and retention of provenance
- **Retrieval,** how to retrieve, explore, and analyze large amounts of collected provenance
- **Scalability,** provenance collection from concurrent large-scale scientific workflows will require a scalable solution
- **Dynamic interference,** provide real-time monitoring and analysis to support runtime workflow steering
- **Context**, integrate system level data to extend provenance descriptions
- **Provenance by Design,** provenance disclosure designed for workflow domain objectives:
  - *Reproducibility, Results Explanation, Performance Optimization, Anomaly Detection, Monitoring, Others…*

Provenance Environment (ProvEn) Services Overview

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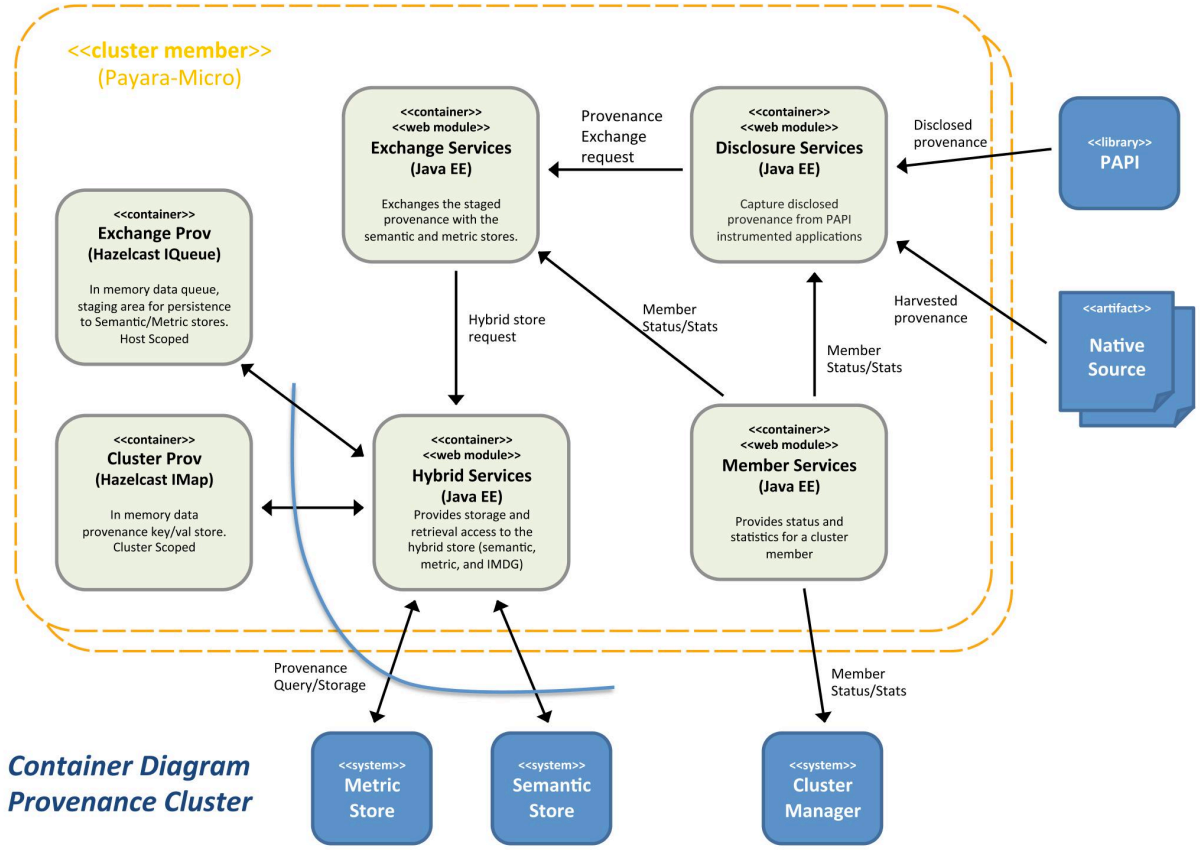
- **ProvEn** is a provenance management platform consisting of loosely coupled components supporting the disclosure, storage, and access to provenance information.

- ***Producer API (PAPI)***
  - ProvEn's provenance disclosure library. Scientific workflow applications instrumented with PAP can produced and disclose their provenance data.

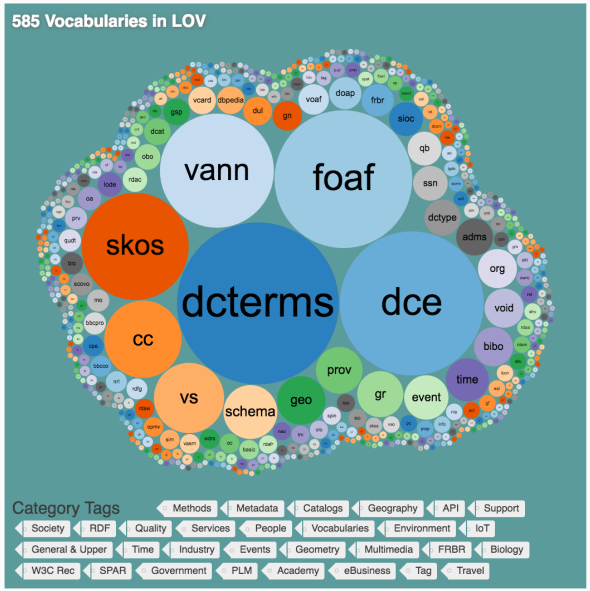
- ***Provenance Cluster***
  - ProvEn's scalable approach for collecting concurrent provenance data streams from PAPI sources.

- ***Hybrid Store***
  - ProvEn combines system level metrics (**Metric Store**) with the traditional disclosed provenance (**Semantic Store**) to create an extended provenance view.



Standards-based Provenance

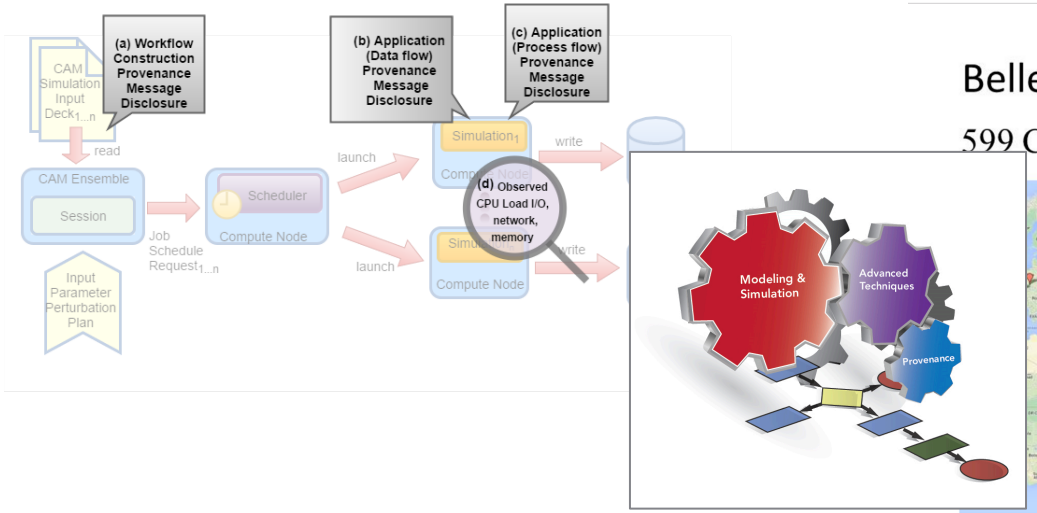
- **W3C PROV** data model published in 2013 defines a core data model for provenance for building representations of the entities, people and processes involved in producing a piece of data or thing in the world.
- **Workflow Performance Provenance** (WFPP) data model is an extension to PROV that will enable the empirical study of workflow performance characteristics and variability including complex source attribution.
- **Provenance Environment** (ProvEn) data model provides concepts specific to the ProvEn provenance management software platform.
- **Domain Specific Descriptive** integration



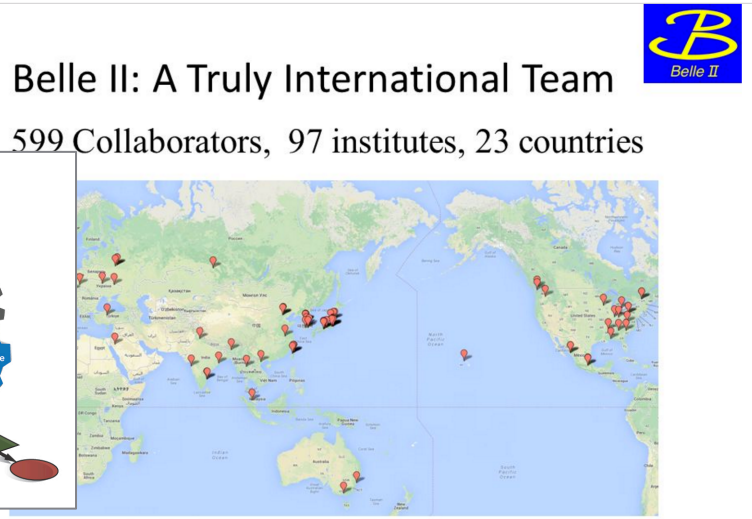
JSON-LD

Research Focus

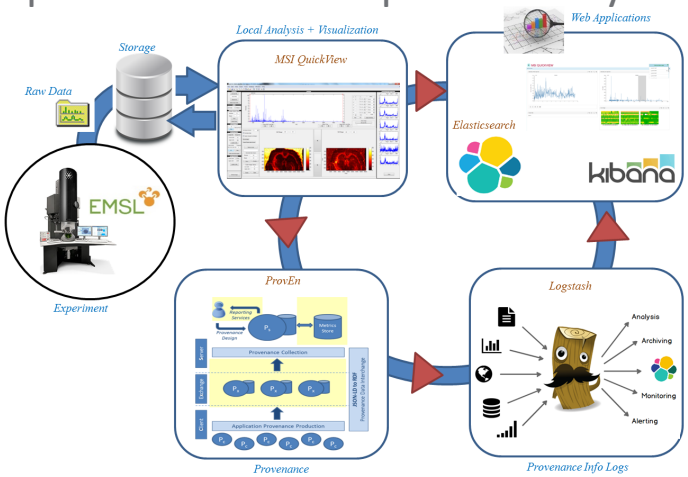
ACME Results Explanation and Performance Tuning



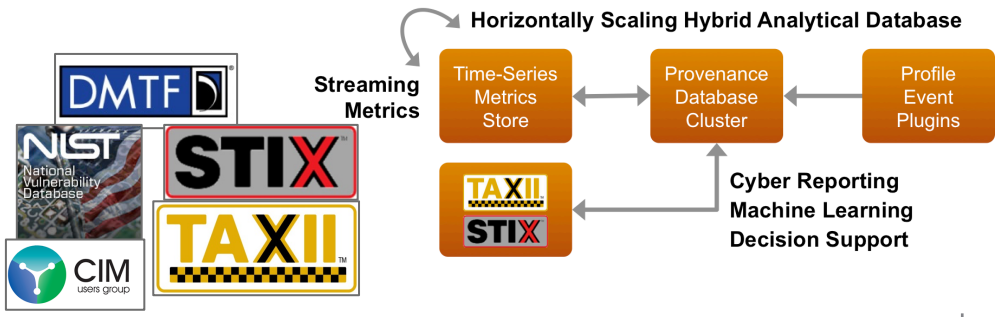
Scheduler Optimization on Belle II



Reproducible Mass Spectrometry Workflows

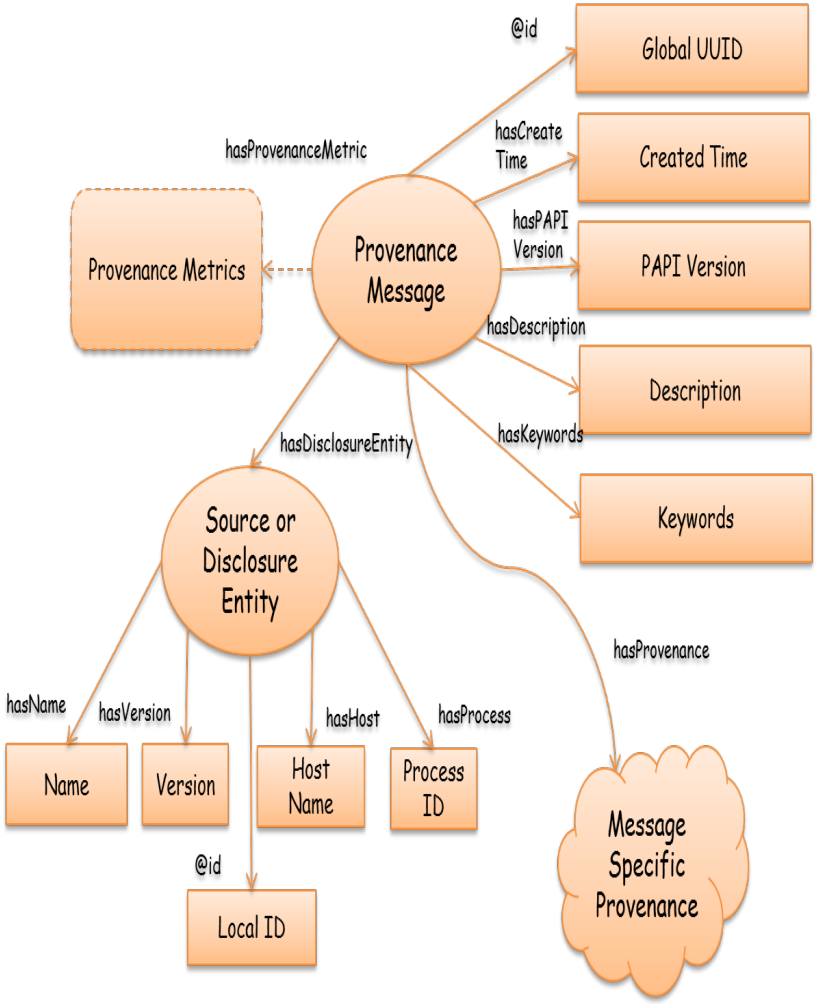


Model Federation and Message Profile Tool Chains



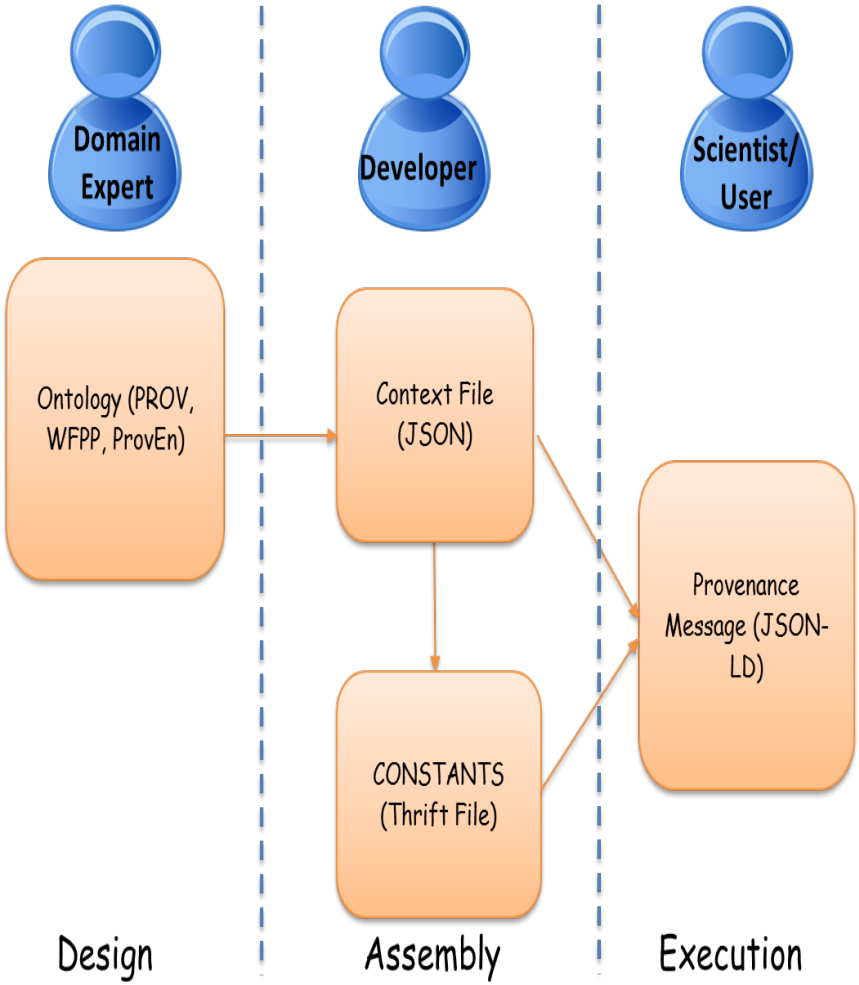
Provenance Message

- **Provenance Message**
  - PAPI's "unit of" provenance
  - Each message is a fragment of the complete provenance graph
  - Every message created uses the same structure (*Header* + *Body*)
  - Provenance by design – messages tailored per PAPI distribution. Ad-hoc also supported
  - Messages are serialized as JSON-LD for a direct interchange to Semantic Store – RDF Database
  - Offline messaging capability

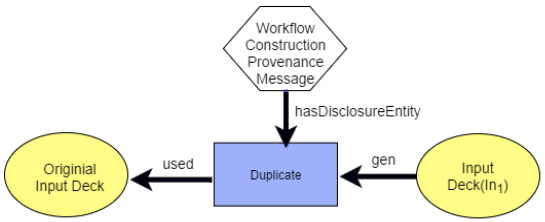


Lifecycle of Provenance Message

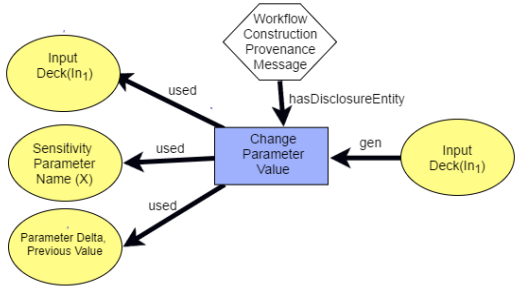
- Provenance Message Design
  - Involves domain expert to identify the provenance messages to support experimental design
  - Uses foundation ontology (e.g. W3C PROV, ProvEn) and domain ontology(WFPP)
- Assembly
  - A domain specific provenance context file is created based on the identified ontological concepts. Enumerated constants are generated for compile time checking
- Message Creation
  - PAPI generates provenance messages based on context file and are serialized into JSON-LD.



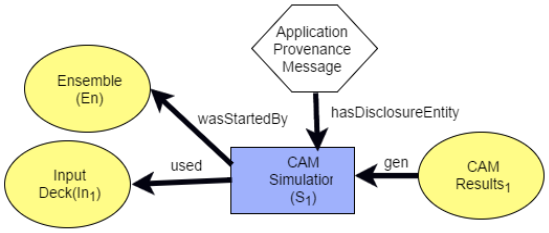
ACME - Message Disclosure and Collection



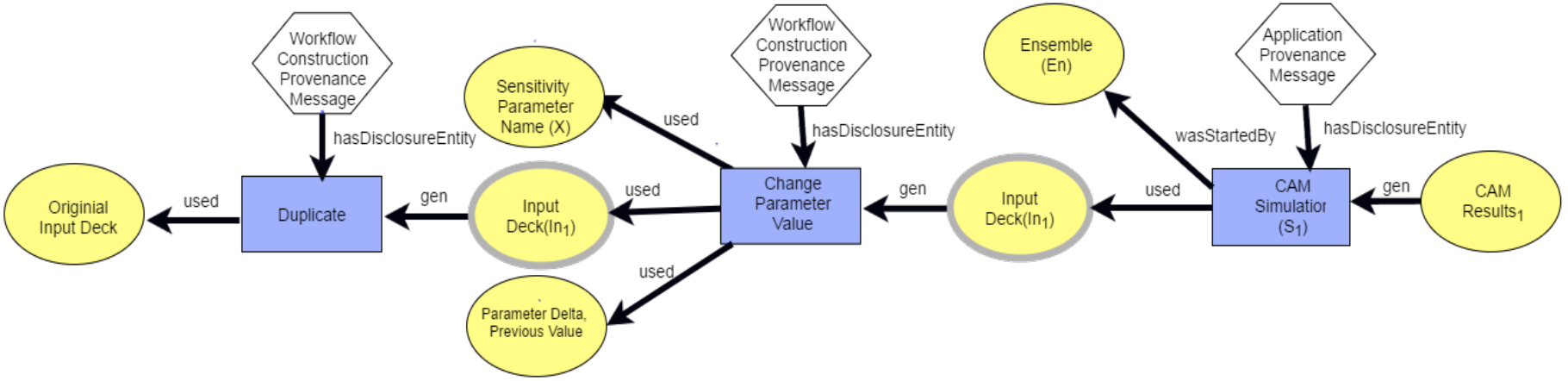
Input Deck Message



Perturbation Message



Results Message



When collected by ProvEn provenance message fragments are integrated into a connected provenance graph to answer the questions posed earlier. The gray outline on entity ovals indicates where messages are connected to form the complete provenance graph.

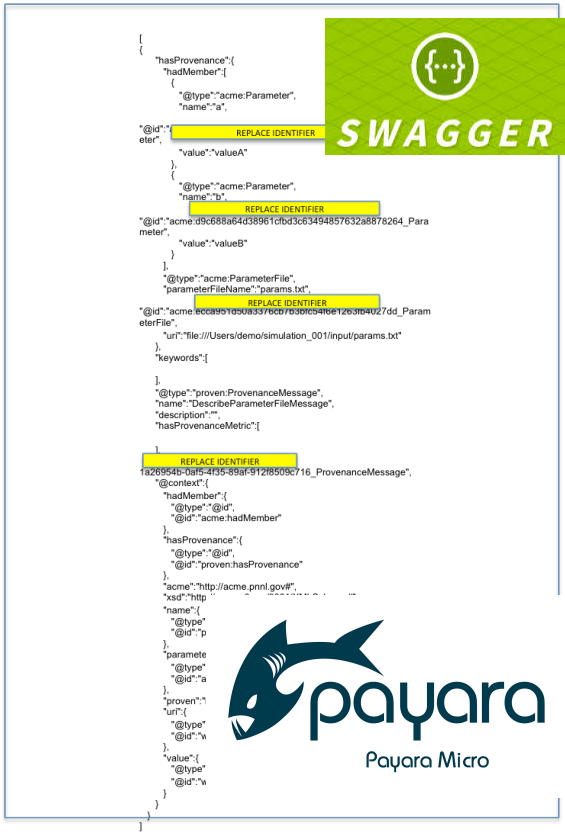
Provenance Disclosure Strategies

- Collecting only relevant information that is used to answer direct questions.

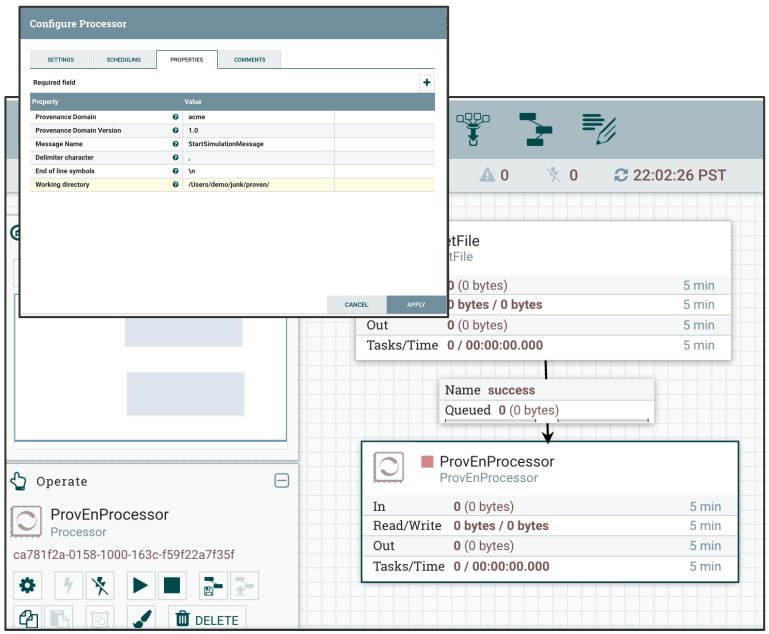
Provenance API (PAPI) calls from standalone or distributed apps

```
…
ProvenanceMessage pm = createMessage(START_APPLICATION);
pm.sendMessage();
…
```

JSON-LD Lightweight REST API



PAPI enabled Harvesting



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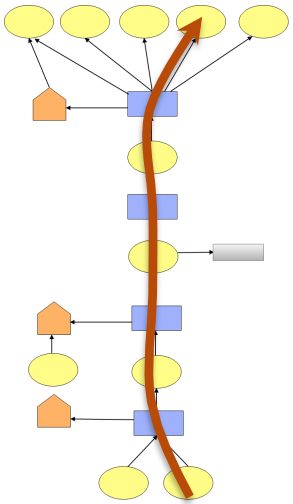
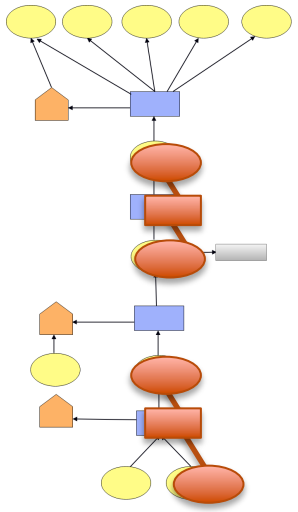
Types of Querying

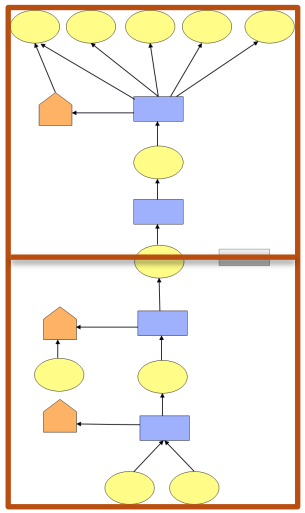
- Regular Expression searches
- Searches
  - Semantic
  - Time-series
- Tracing origin
- Detecting repeating patterns
- Semantic reasoning



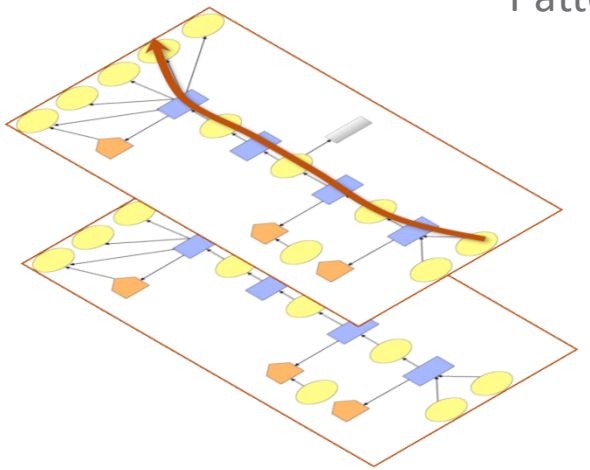
Tracing Data Origin



Detecting Repeating Patterns in subgraphs



Sub-graph partitioning

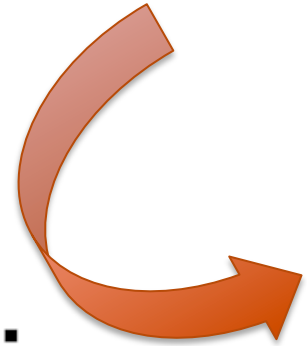


Domain and foundation multi-layer searches

Hybrid Store
What are Provenance Metrics?

- **Provenance Metrics** are discrete pieces of semantic provenance (a single triple) identified in a Provenance Message, and serialized into a time-series format for storage in a registered Metric Store.
- Occurs at time of disclosure, at a minimum alignment of data is by time

```
acme:simulation_1 wfpp:hasStartTime "1471355953002"^^xsd:dateTime
acme:simulation_1 wfpp:hasStopTime  "1471355959001"^^xsd:dataTime
```



timestamp	node	sensor	value	state	message_id	app_id
1471355953002				START	1	1
1471355953004	pi06	CPU1	9.062			
1471355953004	pi06	MEM1	2.464			
1471355953004	pi06	CPU2	8.057			
1471355953004	pi06	MEM2	2.597			
…						
1471355959001				STOP	100	1
…						

ESGF Questions

- How will your efforts help the ESGF community of users?
  - As an active member of standards communities we can both represent needs and notify the ESGF of trends and solutions emerging from any synergistic technological efforts.
  - ProvEn Services
    - As an analytical platform, ProvEn could be used as an integration point for provenance inter-comparison or runtime analytics.
    - As a repository, ProvEn could be hosted by those who lack a provenance solution.
  - PAPI Java client API
    - Used standalone or integrated as a client to ProvEn Services.
  - Working with ESGF to standardize what provenance analytics means for climate science and what disclosures are required to answer priority questions.

ESGF Questions

- What is your timeline for releasing your efforts?
  - We plan to deploy ProvEn in Docker in FY2017.
  - We are in the process of making ProvEn Services and PAPI open source (possibly Spring 2017)
  - Limited deployments could be supported as early as February.
- What standards and services need to be adopted within the environment that will allow ESGF to participate in early adoption?
  - Minimum is dedication of linux box
  - Determining provenance requirements.
- How are you funded for longevity?
  - FY2017 funding on IPPD and ACME.

Acknowledgements

- Todd Elsethagen, Bibi Raju, Malachi Schram, Matt MacDuff, Darren Kerbyson - Pacific Northwest National Laboratory
- Kerstin Kleese van Dam - Brookhaven National Laboratory
- Ilkay Altintas, Alok Singh - San Diego Supercomputer Center & University of California, San Diego

- Project Acknowledgements
  - Integrated End-to-end Performance Prediction and Diagnosis for Extreme Scientific Workflows (IPPD) Project. IPPD is funded by the U. S. Department of Energy Awards FWP-66406 and DEC0012630
  - Accelerated Climate Modeling for Energy (ACME) project funded by the Office of Biological and Environmental Research (BER) in the U.S. Department of Energy (DOE) Office of Science.
  - Analysis In Motion (AIM) Initiative at Pacific Northwest National Laboratory (PNNL), which is conducted under PNNL's Laboratory Directed Research and Development Program

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